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AD-A059078

TOXIC POINT DETERMINATION OF SELECTED HAZARDOUS MATERIALS

LEVEL

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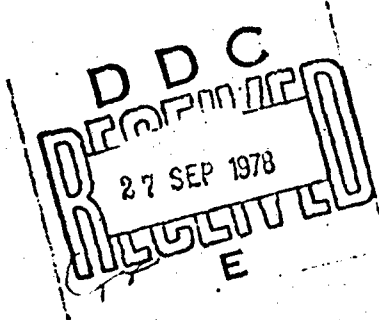
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DEPARTMENT OF TRANSPORTATION
MATERIALS TRANSPORTATION BUREAU
Office of Hazardous Materials Operations
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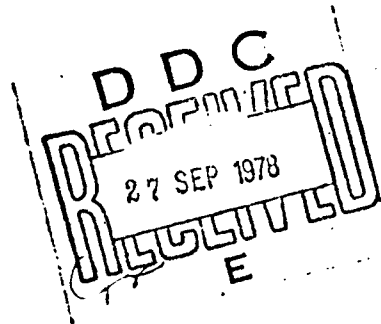
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<p>16. Abstract</p> <p>"Toxic Point" is a term under consideration by the United Nations of Rapporteurs on the Packaging of Dangerous Goods. It is defined the temperature at which the equilibrium concentration of vapor of substance measured at 760 millimeters is equal to the LC50 of the substance. This is also referred to as the "Temperature Threshold Toxicity"</p> <p>This report contains the "Toxic Points" calculated for 57 substance. The calculations are shown together with the toxicity and vapor pressure data used therein.</p>																														
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INTRODUCTION

This report contains the toxic points for 57 of the 85 compounds requested by the Department of Transportation, Materials Transportation Bureau. An extensive search was conducted to obtain vapor pressure and one-hour rat LC₅₀ data. There were many compounds for which no usable rat inhalation toxicity data (LC₅₀'s) could be found. Consequently, other available rat LD₅₀ data were used to estimate an LC₅₀ figure while taking into account the route of administration. When such information was not available for the rat, LC₅₀ or LD₅₀ values from other species were used. The toxic points computed from rat data are listed in Table I. The toxic points computed for other species are listed in Table II.

A toxic point determination was not possible for the following compounds due to unavailable vapor pressure or toxicity information.

No Vapor Pressure Data

Allylamine
Chloroacetaldehyde
4-chloro-o-toluidine Hydrochloride
Diallyl Ether
Diethylenetriamine
Ethylchloroformate
Ethyleneimine
Hexaethyltetraphosphate
Methacrylaldehyde
Methylchloroformate
Methyl Chloromethyl Ether or
Chloromethyl Methyl Ether
Perchloromethylmercaptan

No Toxicity Data

Allyl Ethyl Ether
Antimony Pentafluoride
Arsenic Trichloride
Benzotrichloride
Bromoacetone
Chloroacetone
Chloroprene
Cyanogen Bromide
Diphenylchloroarsine
Ethylchloroarsine
Methyl Bromide
Nitroanisole
Nitrobenzotrifluoride
Nitrobromobenzene
Nitroxylenes
Pentachloroethane
Phenetidine
1,1,2,2-Tetrachloroethane
Xylol Bromide

METHODS

Estimation of The One-Hour LC₅₀

The one-hour rat LC₅₀ was estimated from a rat LC₅₀ of different duration by multiplying the different duration LC₅₀ by the factor $\frac{\text{duration (hours)}}{1 \text{ hour}}$. If no rat LC₅₀ could be found, a rat LD₅₀ was used to calculate an estimated one hour LC₅₀ using the equation shown below:

$$\text{Estimated LC}_{50} = \frac{\text{LD}_{50} \text{ (mg/Kg)} \times \text{Average Rat Body Weight (0.2 Kg)}}{\text{Avg Rat Min Vol (10}^{-4}\text{m}^3\text{/min)} \times 60 \text{ Min} \times \text{Absorption Factor (0.5)}}$$

The units of the estimated LC₅₀ are mg/m³ which are converted to parts per million (ppm) using the formula:

$$\text{ppm (by volume)} = \frac{24.45 \times \text{mg/m}^3}{\text{Molecular Weight}}$$

The vapor pressure equations described below require that the LC₅₀ be expressed as a vapor pressure in millimeters mercury (mm Hg). This was done using the following equation:

$$\text{mm Hg} = \frac{\text{ppm}}{10^6} \times 760$$

Calculation of Toxic Points

Toxic points were calculated by substituting the vapor pressure in mm Hg which corresponded to the one-hour rat LC₅₀ into one of the following equations:

$$1. \text{Log}_{10} P = - \frac{0.2185 A}{T} + B$$

where P is the vapor pressure in mm Hg
T is the temperature in degrees Kelvin
A is the molar heat of vaporization in calories per gram mole
B is a constant

$$2. \text{Log}_{10} P = A - \frac{B}{t + c}$$

where P is the vapor pressure in mm Hg
t is the temperature in degrees centigrade
A, B and C are constants

If the values for A, B and C could not be found for one of these equations, then the constants for equation 2 were calculated. The preferred method of calculating A, B and C was described by Thomson (Chemical Reviews 38:1-39, 1946) and requires the temperature and pressure of three widely separated boiling points. The equations used are as follows:

$$\frac{y_3 - y_2}{y_2 - y_1} \times \frac{t_2 - t_1}{t_3 - t_2} = 1 - \frac{t_3 - t_1}{t_3 + C}$$

$$B = (t_1 + C)(t_3 + C) \times \frac{y_3 - y_1}{t_3 - t_1}$$

$$A = y_1 + \frac{B}{t_1 + C}$$

where: y_1 , y_2 and y_3 equal $\text{Log } P_1$, $\text{Log } P_2$ and $\text{Log } P_3$, respectively; P representing the pressures (mm Hg) at which the different boiling points occur. t_1 , t_2 and t_3 are the temperatures in degrees centigrade of the different boiling points.

If the boiling points are inaccurate or not widely separated, the calculated value of C can be in considerable error and not usable. In this case C was calculated from the equation

$$C = 239 - 0.19t_{760}$$

where t_{760} is the boiling point at 760 mm Hg pressure in degrees centigrade. If only two boiling points could be found for a compound, the value of C was set at 230.

Whenever the values for A, B and C had to be calculated, the values were checked by showing that equation 2 produced the same temperatures and pressures of the boiling points used to calculate A, B and C.

TABLE I
TOXIC POINTS DERIVED FROM RAT DATA

COMPOUND	TP	LC ₅₀		BP		VAPOR PRESSURE CONSTANTS			
	°C	PPM	REF.	°C	REF.	A	B	C	REF.
Cyanogen Chloride	-144.8	59	4a	12.7	12	5243.4	7.541733		12
Nickel Carbonyl	-115.5	17	1a	43.0	11	7021.2	7.738785		12
Chlorine Trifluoride	-110.4	380	1	11.8	11	5932.4	7.436405		12
Acrolein	-97.2	32	1a	52.5	11	7.00995	1175.6	232.2	9*
Ammonia (Anhydrous)	-96.8	7338	1	-33.4	11	7459.6	9.997400		12
Hydrogen Fluoride	-94.9	1276	4	19.7	11	6018.2	7.370000		12
Boron Trichloride	-83.8	3480	13	12.5	11	6165.6	7.543306		12
Nitrogen Tetroxide	-72.6	115	1	8.1	10	†			10
Iron Pentacarbonyl	-65.6	56	1a	103.0	11	8985.8	8.067387		12
Bromochloromethane	-61.4	465	2	68.1	6	6.86624	1132.3	216	6
Methylhydrazine	-48.1	296	4a	87.5	7	7.39188	1403.1	222.4	7*
Acrylonitrile	-44.2	2434	4c	78.5	8	7941.4	7.851016		12
Propionitrile	-40.0	947	4f	97.1	8	8769.0	8.079473		12
Ethyl Bromide	-36.5	26980	1	38.4	8	6843.1	7.635277		12
Chloroform	-35.4	9026	4f	61.3	8	7500.5	7.735083		12
Methylene Chloride	-28.7	33868	4f	40.7	8	7572.3	8.183300		12
Chloropicrin	-20.4	2053	4f	112.0	11	9109.7	8.072388		12
Ethylene Dibromide	-19.9	689	3	131.4	6	7.06245	1469.7	220	6
1,1,2,2-Tetrachloroethylene	-18.6	1624	2f	120.8	8	9240.5	8.026207		12
Allyl Alcohol	-17.7	1620	1	96.5	8	10577.7	9.143231		12
Epichlorohydrin	-17.3	1316	4f	117.9	8	9815.4	8.388568		12
1,1,1,2-Tetrachloroethane	-14.3	1605	4f	130.5	8	9296.5	7.938042		12
Carbon Tetrachloride	-13.6	19056	1	76.6	8	7628.8	7.586045		12
Hydrazine	-5.3	2280	4a	113.5	7	7.55350	1551.4	217.4	7*
Ethylenechlorohydrin	-3.3	1408	4c	128.8	8	10740.6	8.730379		12
Isothio-Cyanic Acid Allyl Ester	5.4	2013	4f	150.7	8	9967.8	8.007150		12

TABLE I (Continued)
TOXIC POINTS DERIVED FROM RAT DATA

COMPOUND	TP	LC ₅₀		BP		VAPOR PRESSURE CONSTANTS			
	°C	PPM	REF.	°C	REF.	A	B	C	RE
Trichloroethylene	12.1	50434	4f	87.2	8	8314.7	7.956342		1
Dichloroethyl Ether	13.6	710	4f	178.0	11	11376.8	8.405945		1
Pyridine	17.3	16000	4a	115.2	8	9649.4	8.347670		1
Aniline	23.2	1000	1a	184.4	8	11307.6	8.221995		1
Dimethyl Sulfate	25.8	1066	4b	188	11	7.629081	1974.6	230	1
Acetonitrile	26.5	124724	4f	81.6	11	8173.2	7.938662		1
Mesityl Oxide	28.9	15382	4f	129.8	8	10109.4	8.383703		1
Toluene Diisocyanate (TDI)	34.8	56	4a	251.0	11	8.11948	2519.8	230	1
Ethylenediamine	36.4	32000	4a	116.5	11	7.91721	1777.8	235.8	
1,2-Dichlorobenzene	39.8	4579	3f	179.0	8	10943.0	8.185275		1
Ester Isocyanophenyl	45.1	10632	4f	165.6	8	10556.7	8.159059		1
2-Chlorophenol	46.4	9960	4c	174.5	8	10341.1	7.952334		
Ethyl Sulfate (Diethyl)	59.7	2974	4b	208.0	12	12518.2	8.574200		
1,2,4-Trichlorobenzene	64.3	5605	4f	213.0	8	11425.1	8.030523		
1,4-Dichlorobenzene	66.3	22908	4e	173.9	6	10611.0	8.073632		
Acetocyanohydrin	66.8	248	1a	95.0	11	39.6536	11620.2	221	
Benzonitrile	72.9	15671	4d	191.3	8	11341.0	8.239760		
Chloronitrobenzene (Ortho)	75.2	2461	4f	245.5	11	7.55514	2222.6	230	
o-Toluidine	79.4	11316	4f	199.8	8	12663.4	8.785945		
m-Toluidine	81.0	12237	4f	202.9	8	12104.1	8.440371		
Nitrotoluene (Ortho)	85.3	8750	4f	220.4	8	12239.1	8.286642		
p-Toluidine	86.2	16145	3f	200.4	8	12428.6	8.648585		
Benzylidene Chloride	96.1	27184	4f	214.0	8	11075.9	7.871695		
Diethylaniline	105.7	24263	4f	216.3	8	12539.2	8.501130		

TABLE I (Continued)
TOXIC POINTS DERIVED FROM RAT DATA

1. * - Vapor pressure constants mathematically derived from boiling points.
2. The following letters indicate an estimated one-hour LC₅₀ and the type of data on which it is based. Numbers indicate the reference source.

a = inhalation duration other than one hour
b = intravenous LD₅₀
c = subcutaneous LD₅₀
d = skin LD₅₀
e = intraperitoneal LD₅₀
f = oral LD₅₀

3. † - The equation used to calculate the TP of nitrogen tetroxide was

$$\ln P = 32.1662156 - \frac{7788.62341}{T} + \frac{172043.271}{T^2}$$

TABLE II
TOXIC POINTS DERIVED FROM OTHER THAN THE RAT DATA

COMPOUND	TP	LC ₅₀		BP		VAPOR PRESSURE CONST		
	°C	PPM	REF.	°C	REF.	A	B	
Allylchloride (M)	-62.7	2734	4e	44.6	8	7386.8	7.991952	
Carbon Disulfide (R)	-58.0	5303	2c	46.5	11	6786.8	7.502434	
Butyrenitrite (R)	8.7	9737	4d	117.5	8	9462.9	8.207895	
Methylchloroform (GP)	14.3	95618	4f	74.1	8	8012.7	7.955902	
Carbon Tetrabromide (M)	20.5	1211	4c	107.5	8	10771.4	7.983739	
Bromoform (M)	28.8	9697	4c	150.5	8	7.30383	1720.6	22
Acetylene Tetrabromide (GP)	67.5	1553	4f	240.5	12	12911.5	8.357191	

1. * - Vapor pressure constants mathematically derived from boiling points..

2. The following letters indicate an estimated one-hour LC₅₀ and the type of data on which it is based. Numbers indicate the reference source..

a = inhalation duration other than one hour
b = intravenous LD₅₀
c = subcutaneous LD₅₀
d = skin LD₅₀
e = intraperitoneal LD₅₀
f = oral LD₅₀

3. (M) = Mouse
(R) = Rabbit
(GP) = Guinea Pig

REFERENCES

1. Back, K.C., Thomas, A.A., and MacEwen, J.D.; Reclassification of Materials Listed as Transportation Health Hazards, Report No. TSA-20-72-3, 6570th Aerospace Medical Research Laboratory (AFSC), Wright-Patterson Air Force Base, Ohio; August 1972.
2. Christensen, H.E. and Luginbyhl, T.T.; The Toxic Substances List 1973 Edition, U. S. Department of Health, Education and Welfare, National Institute for Occupational Safety and Health, Rockville, Maryland; June 1973.
3. Christensen, H.E. and Luginbyhl, T.T.; The Toxic Substances List 1974 Edition, U. S. Department of Health, Education and Welfare, National Institute for Occupational Safety and Health, Rockville, Maryland; June 1974.
4. Christensen, H.E. and Luginbyhl, T.T.; Registry of Toxic Effects of Chemical Substances, U. S. Department of Health, Education and Welfare, National Institute for Occupational Safety and Health, Rockville, Maryland; June 1975.
5. Dreisbach, R.R.; Pressure - Volume - Temperature Relationships of Organic Compounds, 3rd Edition, Handbook Publishers, Inc.; 1952.
6. Dreisbach, R.R.; Physical Properties of Chemical Compounds, Volume II, Advances in Chemistry Series Volume 22; 1959.
7. JANNAF Hazards Working Group; Chemical Rocket/Propellant Hazards Volume III. Liquid Propellant Handling, Storage and Transportation, Chemical Propulsion Information Agency, Pub. No. 194,; May 1970.
8. Jordan, T.E.; Vapor Pressure of Organic Compounds, Interscience Publishers, Inc., New York; 1954.
9. Perry, R.R. and Chilton, C.H.; Chemical Engineers' Handbook, 5th Edition, McGraw-Hill Book Company; 1973.
10. Saraceno, O.J. and Willis, C.D.; Vapor Pressure - Temperature Data for Selected Halogen-Containing Substances, Goodyear Atomic Corporation, Piketon, Ohio; February 1971.
11. Stecher, P.G.; The Merck Index, Merck and Company, Inc.; Rahway, New Jersey, 1968.
12. Weast, R.C.; Handbook of Chemistry and Physics, 53rd Edition, The Chemical Rubber Company, Cleveland, Ohio; 1972.
13. Unpublished Data - Toxic Hazards Research Unit, University of California.

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